

Kamlet-Taft Parameters and Predictive Models for the Design and Selection of Alternative Supercritical Fluid Solvents

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The research in our group has focused on the measurement and modeling of specific interactions in solvent-solute systems. Perhaps the most well known set of solvent and solute descriptors are the Kamlet-Taft parameters. These parameters provide numerical values for three important solvent and solute interactions; dipolarity-polarizability, hydrogen-bond donor ability, and hydrogen-bond acceptor ability. Historically, scales of these parameters have been established to allow for qualitative intercomparison of solvent and solute properties. These parameters can also be used quantitatively in modeling solution equilibrium in the form of a linear solvation energy relationship (LSER). Our experimental results include measurement of the Kamlet-Taft solvent parameters for six fluorinated ethanes over gas, supercritical fluid, and liquid densities. The measured ultraviolet electronic transitions of the solvatochromic probe molecules in a given fluorinated solvent were fitted to third-order polynomials in solvent density for all isotherms investigated. Values for the Kamlet-Taft parameters were calculated for each of the solvents as a function of the solvent density. Trends in the measured Kamlet-Taft parameters were related to the degree of fluorination on the ethane molecule. We have used the measured Kamlet-Taft parameters and Abraham's solute descriptors as independent variables in an LSER to model our measurements of the supercritical fluid-water partitioning of organic solutes. Systems studied include HFC134a-water, HFC143a-water, and carbon dioxide-water. Additionally, we have measured the Kamlet-Taft parameters of two additional solvent classes, the glycol ethers and alkanol amines.